

# Physics of iron-based high temperature superconductors

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## Abstract

The discovery of high- $T_c$  iron pnictide and chalcogenide superconductors has been one of the most exciting recent developments in condensed matter physics. Although there is general consensus on the unconventional pairing state of these superconductors, several central questions remain, including the role of magnetism and orbital degrees of freedom and the resultant superconducting gap structure. The search for universal properties and principles continues. Here I review the recent progress of research on iron-based superconducting materials, highlighting the important questions that remain to be conclusively answered.

In 2006, Hideo Hosono's research group found superconductivity below 6 K in LaFePO [1]. They discovered that by replacing phosphorus with arsenic and doping the structure by substituting some of the oxygen atoms with fluorine they could increase  $T_c$  up to 26 K [2]. This high  $T_c$  in LaFeAs(O,F) aroused great interest in the superconducting community, particularly when it was found that  $T_c$  could be increased up to 43 K with pressure. By the end of April 2008, it was found that  $T_c$  could be increased to 56 K by replacing La with other rare earth elements. Thus iron-pnictides joined the cuprates and became a new class of *high- $T_c$*  superconductor.

The most important aspect of the iron-pnictides may be that they open a new landscape in which to study mechanisms of unconventional pairing which lead to high- $T_c$  superconductivity [3–7]. The high transition temperatures in both cuprates and iron-pnictides cannot be explained theoretically by the conventional electron-phonon pairing mechanism and thus there is almost complete consensus that the origin of superconductivity of both systems has an unconventional origin [7, 8]. Another class of materials in which there is extensive evidence for unconventional superconductivity are the heavy fermion compounds [9]. The unusual properties of these materials originate from the  $f$  electrons in the Ce ( $4f$ ) or U ( $5f$ ) atoms which interact with the conduction electrons to give rise to heavy effective electron masses (up to a few hundred to a thousand times the free electron mass) through the Kondo effect.

There are several notable similarities between these three classes of unconventional superconductor. First of all, it is widely believed that in all three systems electron correlation effects play an important role for the normal-state electronic properties as well as the superconductivity. As in high- $T_c$  cuprates and some of the heavy fermion compounds, superconductivity in iron-pnictides emerges in close proximity to an antiferromagnetic (AFM) order, and  $T_c$  has dome-shaped dependence on doping or pressure. In these three systems near the optimal  $T_c$  composition various normal-state quantities often show a striking deviation from conventional Fermi liquid behavior and its relationship to the quantum critical point has been a hot topics [12, 13].

Structurally, iron-pnictides also have some resemblance to cuprates: pnictides are two dimensional (2D) layered compounds with alternating Fe-pnictogen (Pn) layers sandwiched between other layers which either donate charge to the Fe-Pn layers or create internal pressure. However, there are also significant differences between three systems. For example,

the parent compounds of the iron-pnictides are metals whereas for cuprates they are Mott insulators. Moreover, whereas in cuprates the physics is captured by single band originating from a single  $d$ -orbital per Cu site, iron-based superconductors have six electrons occupying the nearly degenerate  $3d$  Fe orbitals, indicating that the system is intrinsically multi-orbital and therefore that the inter-orbital Coulomb interaction also plays an essential role. Indeed, it is thought that orbital degrees of freedom in pnictides give rise to a rich variety of phenomena, such as nematicity [10, 11] and orbital ordering [14]. In cuprates a crucial feature of the phase diagram is the mysterious pseudogap phase. At present it is unclear if an analogous phase exists in iron-pnictides.

In heavy fermion compounds, the  $f$  electrons, which localize at high temperature, become itinerant at low temperature through Kondo hybridization with the conduction electrons. Heavy fermion compounds usually have complicated 3D Fermi surfaces. The competition of various interactions arising from Kondo physics often makes their magnetic structures complicated. Orbital physics is also important in heavy fermion compounds, as shown by multipolar ordering (this corresponds to orbital ordering in  $d$  electron system), but often its nature is not simple due to the complicated Fermi surface and strong spin-orbit interaction. Iron-pnictides, in sharp contrast, have much simpler quasi-2D Fermi surface with weaker spin-orbit interaction and simple magnetic structures [15].

Listed below are the topics covered in this lecture.

## I. INTRODUCTION

- Why are iron-based superconductors important?
- Are iron-based superconductors unconventional?
- Similarity and differences between cuprates and iron-pnictides

## II. NORMAL STATE PROPERTIES

- Electron correlations, quantum critical point and non-Fermi liquid properties.
- Role of magnetism and orbital degree of freedom

- Nematicity

### III. SUPERCONDUCTING PROPERTIES

- Superconducting gap structure
- Is the major pairing interaction attractive or repulsive;  $s_{\pm}$  or  $s_{++}$ ?
- Nodal gap structure and the presence of two (or more) competing pairing interactions
- BCS-BEC crossover and highly spin-polarized Fermi liquid

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- [1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **128**, 10012-3 (2006).
  - [2] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296-7 (2008).
  - [3] K. Ishida, Y. Nakai, and H. Hosono, J. Phys. Soc. Jpn. **78**, 062001 (2009).
  - [4] J. Paglione and R.L. Greene, Nature Phys. **6**, 645-58 (2010).
  - [5] G.R. Stewart, Rev. Mod. Phys. **83** 1589-652 (2011).
  - [6] I.I. Mazin, Nature **464**, 183-6 (2010)..
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  - [10] R. M. Fernandes, A. V. Chubukov, and J. Schmalian, Nature Phys. **10**, 97?104 (2014).
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  - [12] K. Hashimoto *et al.*, Science **336** 1554 (2012).
  - [13] T. Shibauchi, A. Carrington and Y. Matsuda, Annu. Rev. Condens. Matter Phys. **5**, 113-35 (2014).
  - [14] T. Shimojima *et al.* Phys. Rev. B **89**, 045101 (2014).
  - [15] P. Dai, J. Hu, and E. Dagotto, Nature Phys. **8**, 709-18 (2012).

# Physics of iron-based high temperature superconductors

## 1) Introduction

## 2) Similarities and differences between cuprates and Fe-pnictides

## 3) Normal state properties

Electronic structure, magnetism and orbital degrees of freedom

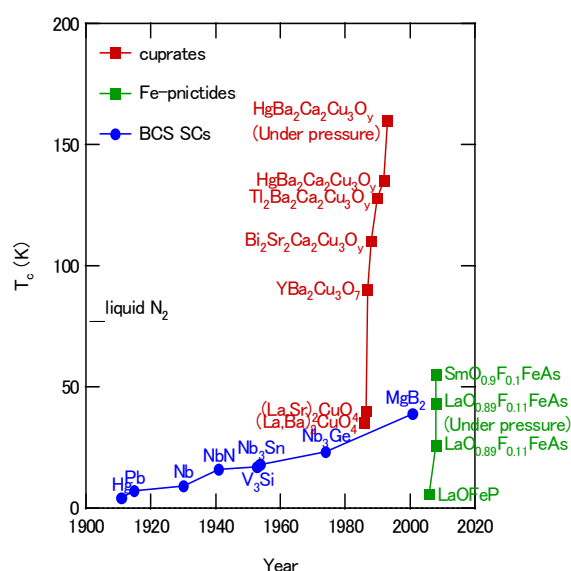
## 4) Superconducting gap structure

Is the major pairing interaction repulsive or attractive?

## 5) Some recent topics

QCP, BCS-BEC crossover, Nematicity••••

## Fe-based high- $T_c$ superconductors



## Why are Fe-pnictides important?

### 1. A new class of high temperature superconductors

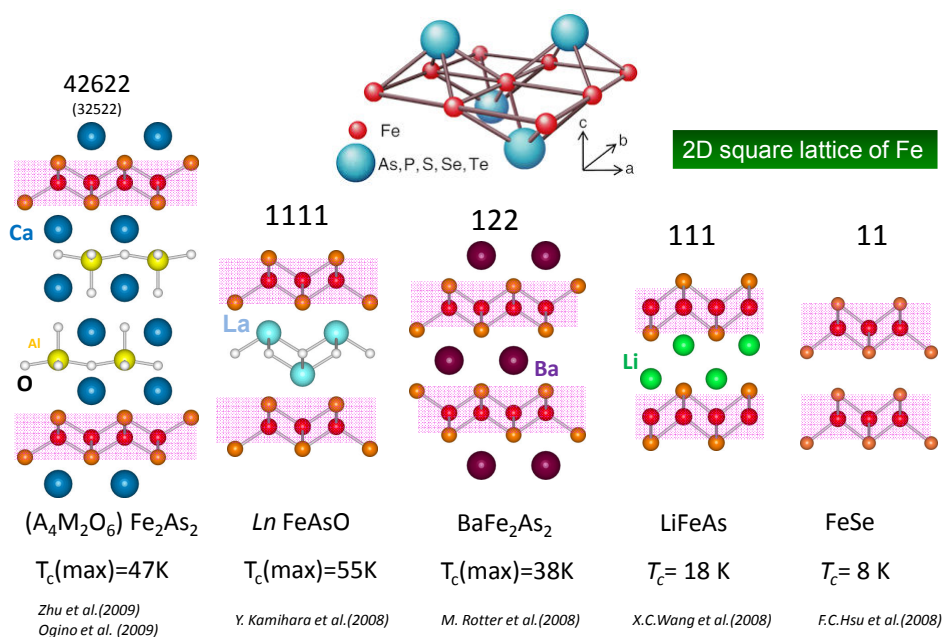
They knocked the cuprates off their pedestal as a unique class of high temperature superconductors.

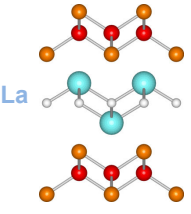
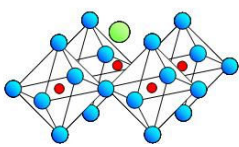
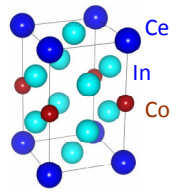
### 2. A new family of unconventional superconductors

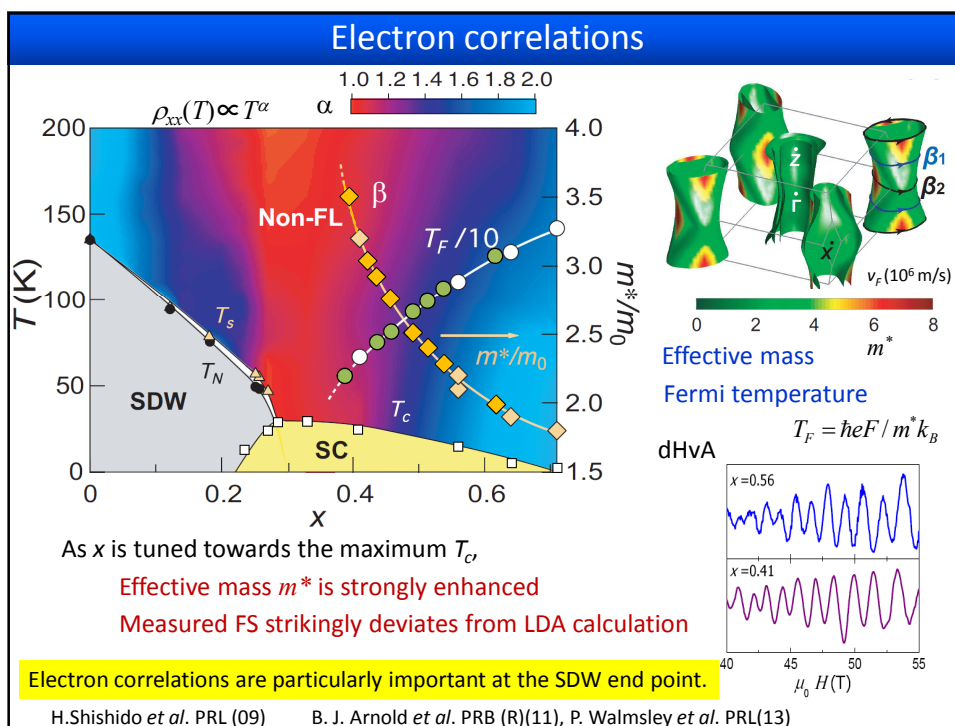
A possible new mechanism of high- $T_c$  superconductivity

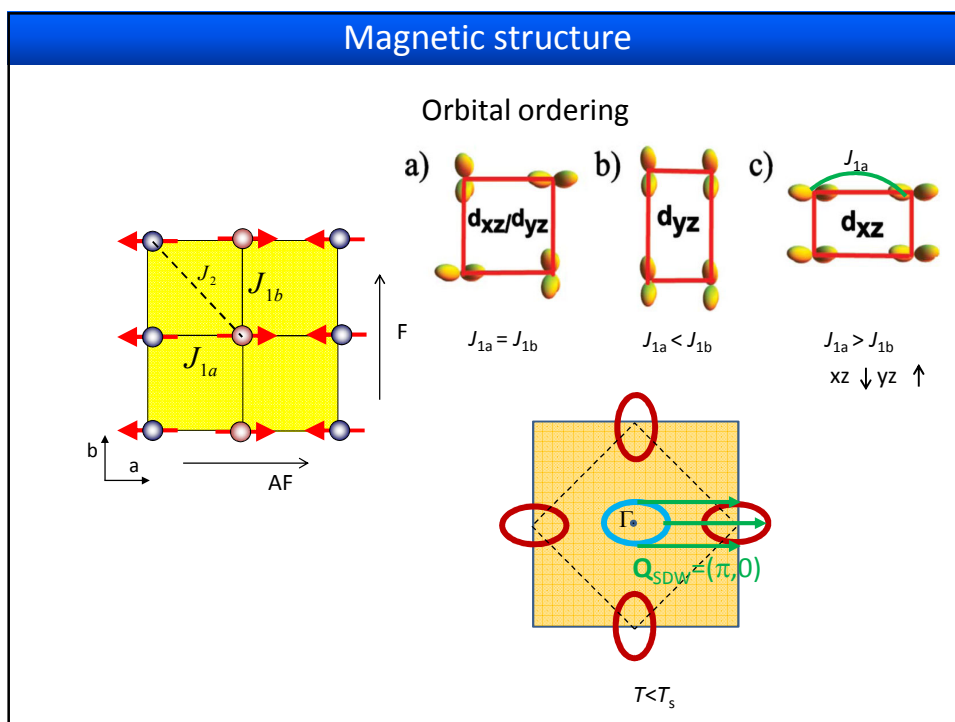
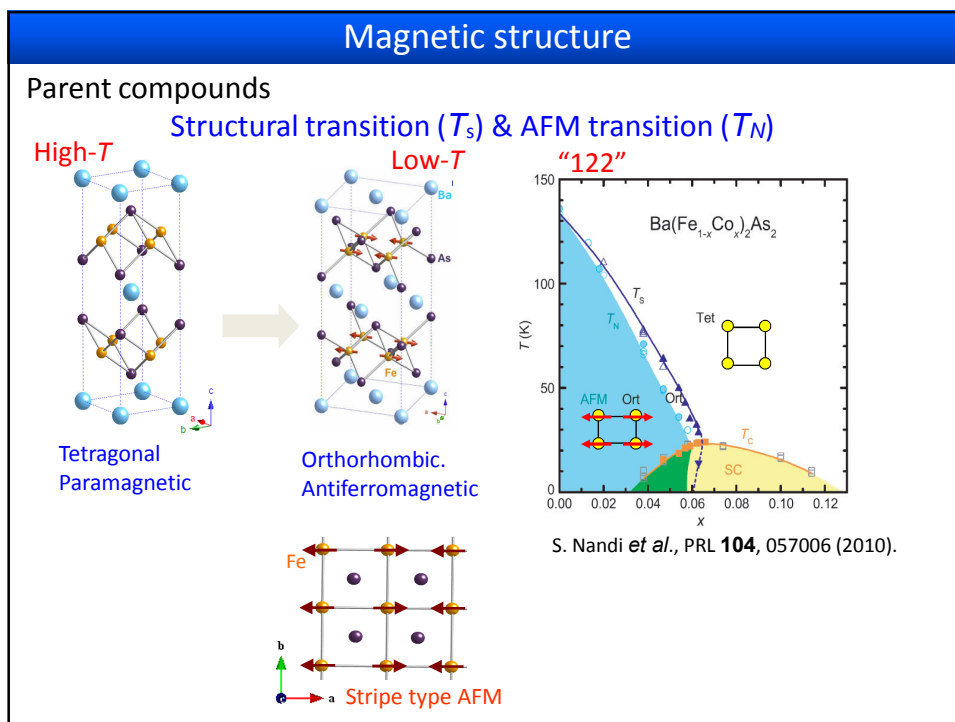
### 3. They would be easier to work into technological applications than the cuprates.

## Fe-based high- $T_c$ superconductors



| Three families of unconventional superconductor                                   |                                                                                   |                                                                                     |                |
|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|----------------|
| Iron pnictide (Fe)                                                                | Cuprate (Cu)                                                                      | Heavy fermion compound (Ce, U)                                                      |                |
|  |  |  |                |
|                                                                                   | Pnictide                                                                          | Cuprate                                                                             | Heavy Fermion  |
| Electron correlation                                                              | strong                                                                            | < strong                                                                            | < very strong  |
| Fermi surface                                                                     | simple 2D                                                                         | Very simple 2D                                                                      | Complicated 3D |
| Magnetic structure                                                                | simple                                                                            | simple                                                                              | complicated    |
| Physics                                                                           | Multi-orbital                                                                     | Mott                                                                                | Kondo          |

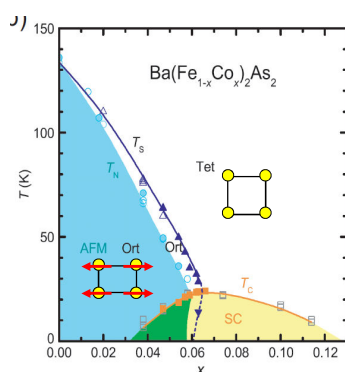




## Relationship between magnetic order and structural transition

Two scenarios

- 1) Orbital ordering triggers stripe SDW order.
- 2) Magnetic interaction (spin nematic) induces orbital order through the spin-lattice coupling.



Structural ( $T_s$ ) and AFM transition ( $T_N$ ) lines follow closely each other

$T_s$ : orbital order

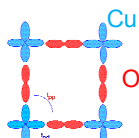
$T_N$ : SDW order



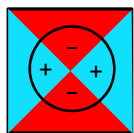
## Iron pnictides: candidate for the SC state

### Cuprates

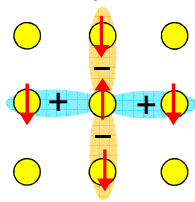
$d_{x^2-y^2}$



$k$ -space (repulsive)

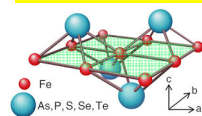


$r$ -space



$$\Delta(\cos k_x - \cos k_y)$$

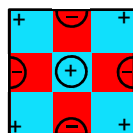
### Fe-pnictides



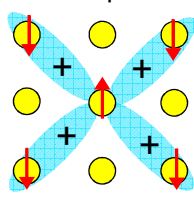
$S_{+-}$

$S_{++}$

$k$ -space (repulsive)

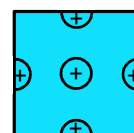


$r$ -space

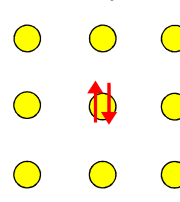


$$\Delta(\cos k_x \cos k_y)$$

$k$ -space (attractive)



$r$ -space



$$\Delta$$

## Iron pnictides: candidate for the SC state

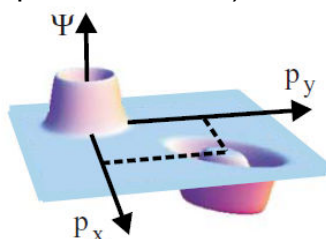
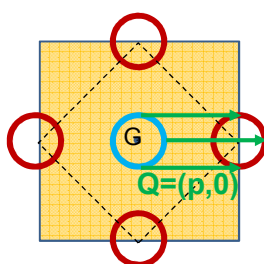
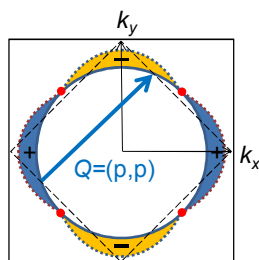
- Pairing due to purely **repulsive** electronic interaction (enhanced by spin fluctuations)

 $S_{+-}$ 

$V > 0$

AFM spin fluctuations

cf. d-wave cuprate



I. I. Mazin et al., PRL 101, 057003 (2008).  
 K. Kuroki et al., PRL 101, 087004 (2008).  
 & PRB 79, 224511 (2009).  
 A. V. Chubkov et al., PRB 80, 140515(R) (2009).  
 S. Graser et al., NJP 11, 025016 (2009).  
 H. Ikeda, PRB 81, 054502 (2010).  
 K. Seo et al., PRL 101, 206404 (2008).  
 F. Wang et al., PRL 102, 047005 (2009).

⋮

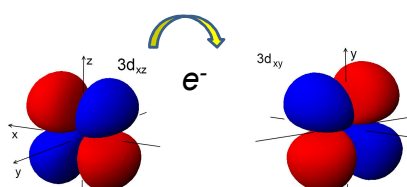
## Iron pnictides: candidate for the SC state

- Pairing due to **attractive** interaction caused by charge/orbital fluctuations.

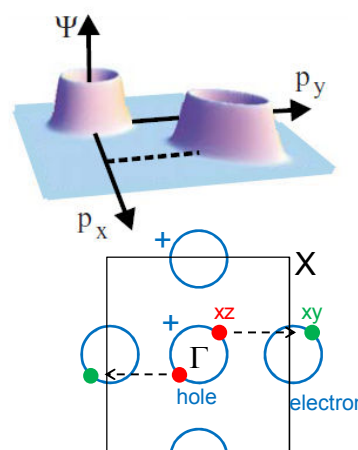
 $S_{++}$ 

$V < 0$

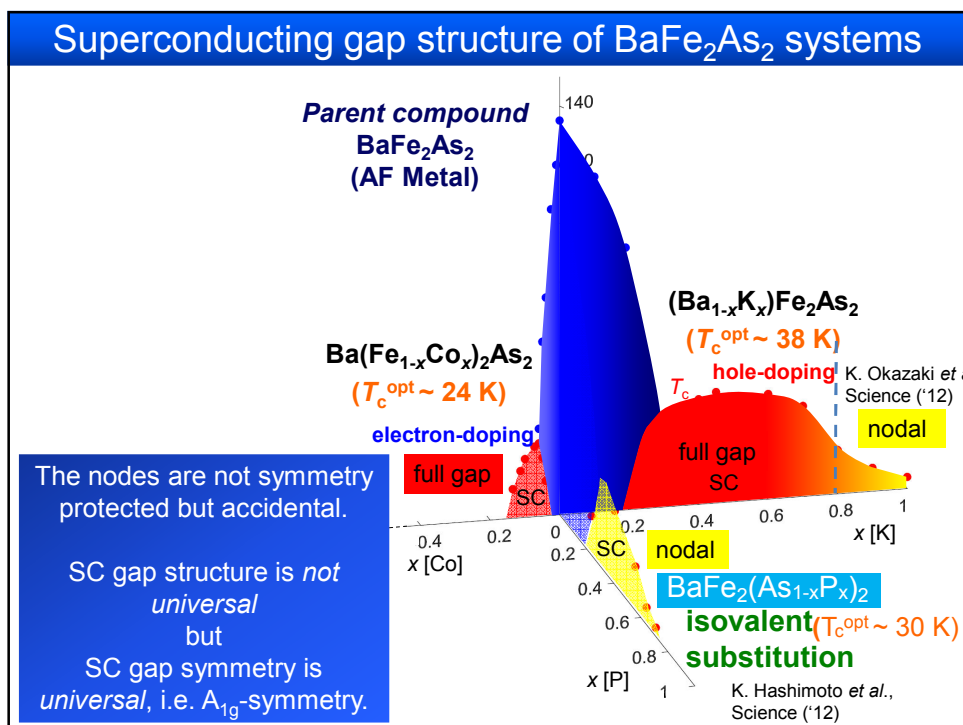
Orbital fluctuations  
(Quadrupole fluctuations)



Charge up  
 Charge down  
 Occupation number of each orbit  
 at each Fe site fluctuates



H. Kontani & S. Onari, PRL 104, 157001 (2010).  
 F. Kruger et al., PRB 79, 054504 (2009).  
 Y. Yanagi et al., PRB 81, 054518 (2010).



### What the gap structure tells us?

**Full gap superconductivity**  
Is the major pairing interaction repulsive or attractive?

$S_{+-}$

Repulsive  
Spin fluctuations

?

$S_{++}$

Attractive  
Orbital fluctuations

?

No conclusive experimental evidence so far

**Some pnictides have line nodes**

Presence of repulsive (magnetic) pairing interaction

Line node is accidental (not symmetry protected)

Presence of two (or more) competing pairing interactions

